INVENTOR SEARCH

=> fil cap1; d que nos 124

FILE 'CAPLUS' ENTERED AT 09:53:37 ON 23 DEC 2008

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FILE COVERS 1907 - 23 Dec 2008 VOL 149 ISS 26 FILE LAST UPDATED: 22 Dec 2008 (20081222/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/legal/infopolicy.html 'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

| L1 | 1 | SEA | FILE=CAPLUS | SPE=ON | ABB=ON | US2006-584440/AP |
|-----|-----|-----|-------------|----------|----------|-----------------------------|
| L5 | | STR | | | | |
| L8 | 129 | SEA | FILE=REGIST | RY SSS F | UL L5 | |
| L9 | | STR | | | | |
| L11 | | STR | | | | |
| L16 | 57 | SEA | FILE=REGIST | RY SUB=L | 8 SSS FU | L (L9 OR L11) |
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| L19 | 0 | SEA | FILE=CAPLUS | SPE=ON | ABB=ON | SHOUTTEETEN A?/AU |
| L20 | 4 | SEA | FILE=CAPLUS | SPE=ON | ABB=ON | BLEGER F?/AU |
| L21 | 2 | SEA | FILE=CAPLUS | SPE=ON | ABB=ON | MORDACQ F?/AU |
| L22 | 67 | SEA | FILE=CAPLUS | SPE=ON | ABB=ON | PIRON J?/AU |
| L23 | 37 | SEA | FILE=CAPLUS | SPE=ON | ABB=ON | SCHOUTEETEN A?/AU |
| L24 | 2 | SEA | FILE=CAPLUS | SPE=ON | ABB=ON | (L1 OR L19 OR L20 OR L21 OR |
| | | L22 | OR L23) AND | L18 | | |

=> d ibib abs hitstr 124 1-2

L24 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2005:569050 CAPLUS <u>Full-text</u>

DOCUMENT NUMBER: 143:97254

TITLE: Process for preparation de
2-(n-alkyl)-3-(4-hydroxybenzoyl)benzofurans and intermediates by halogenation of carboxybenzofuran derivatives, Friedel-Crafts acylation with alkoxybenzenes and dealkylation

INVENTOR(S): Schouteeten, Alain; Bleger, Francois
; Mordacq, Francoise; Piron, Jerome

PATENT ASSIGNEE(S): Clariant France, Fr. SOURCE: Fr. Demande, 22 pp.

CODEN: FRXXBL

DOCUMENT TYPE: Patent. LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PA: | FENT 1 | NO. | | | KINI | D | DATE | | | APPL | ICAT | ATION NO. DATE | | | | | |
|-------|--------------|------|------|-----|------|------|--------------|------|-----|----------|------|----------------|-----|-----|-----|------|-------|
| | 2864 2864 | | | | | | 2005 2006 | | | FR 2 | 003- | 1539 | 8 | | 2 | 0031 | 224 |
| WO | 2005 | 0661 | 49 | | A1 | | 2005 | 0721 | | WO 2 | 004- | IB41 | 58 | | 2 | 0041 | 215 |
| | W: | ΑE, | AG, | AL, | ΑM, | ΑT, | ΑU, | ΑZ, | BA, | BB, | BG, | BR, | BW, | BY, | BZ, | CA, | CH, |
| | | CN, | CO, | CR, | CU, | CZ, | DE, | DK, | DM, | DZ, | EC, | EE, | EG, | ES, | FΙ, | GB, | GD, |
| | | GE, | GH, | GM, | HR, | HU, | ID, | IL, | IN, | IS, | JP, | KE, | KG, | KP, | KR, | KΖ, | LC, |
| | | LK, | LR, | LS, | LT, | LU, | LV, | MA, | MD, | MG, | MK, | MN, | MW, | MX, | MZ, | NA, | NI, |
| | | NO, | NZ, | OM, | PG, | PH, | PL, | PT, | RO, | RU, | SC, | SD, | SE, | SG, | SK, | SL, | SY, |
| | | ТJ, | TM, | TN, | TR, | TT, | TZ, | UA, | UG, | US, | UΖ, | VC, | VN, | YU, | ZA, | ZM, | ZW |
| | RW: | BW, | GH, | GM, | ΚE, | LS, | MW, | MZ, | NA, | SD, | SL, | SZ, | TZ, | UG, | ZM, | ZW, | AM, |
| | | ΑZ, | BY, | KG, | KΖ, | MD, | RU, | ТJ, | TM, | AT, | BE, | BG, | CH, | CY, | CZ, | DE, | DK, |
| | | EE, | ES, | FΙ, | FR, | GB, | GR, | HU, | ΙE, | IS, | ΙΤ, | LT, | LU, | MC, | NL, | PL, | PT, |
| | | RO, | SE, | SI, | SK, | TR, | BF, | ВJ, | CF, | CG, | CI, | CM, | GΑ, | GN, | GQ, | GW, | ML, |
| | | MR, | ΝE, | | TD, | | | | | | | | | | | | |
| EP | 1699 | 772 | | | A1 | | 2006 | 0913 | | EP 2 | 004- | 8013 | 95 | | 2 | 0041 | 215 |
| | R: | ΑT, | BE, | CH, | DE, | DK, | ES, | FR, | GB, | GR, | ΙΤ, | LI, | LU, | NL, | SE, | MC, | PT, |
| | | • | | | | | CY, | | | | | | | | | | |
| | 1898 | | | | | | 2007 | | | | | | | | | | |
| | 2007 | | | | | | | | | | | | | | | | |
| | 2006 | | | | | | | | | | | | | | | 0060 | |
| | 2006 | | | | | | 2006 | | | | 006- | | | | | 0060 | |
| | 2006 | | | | | | 2007 | | | | 006- | | | | _ | 0060 | |
| | 2007 | | | | A1 | | 2007 | 0705 | | | 006- | | | | | | 129 < |
| ORIT: | Y APP | LN. | INFO | .: | | | | | | | 003- | | | | | | |
| | | | | | | | | | | WO 2 | 004- | IB41. | 58 | 1 | W 2 | 0041 | 215 |
| ER SO | DURCE | (S): | | | CASI | REAC | T 14 | 3:97 | 254 | | | | | | | | |

OTHER SOURCE(S): CASREACT 143:97254

GΙ

AB The invention is related to the preparation of benzofurans I [R = linear or]branched alkyl; R1 = halo, NO2, linear or branched alkyl, alkoxy] and intermediates by halogenation of acids II [R1, R defined as above] in an organic solvent, Friedel-Crafts acylation of alkoxybenzenes of formula C6H5OR2 (III) [R2 = linear or branched alkyl] with acyl halides IV (X = halo) in the presence of a Lewis acid to V [R, R1, R2 defined as above] and its 2-alkoxy isomer, and dealkylation. The invention is also related to the preparation of II by heating VI [R1' = NO2; R4 = linear or branched alkyl] and its ketone tautomer in the presence of an acid catalyst. The advantages include absence of poisoned materials, higher yields and purities. For example, chlorination of 2-(n-butyl)-3-carboxy-5-nitrobenzofuran with SOC12 in PhCl, acylation of anisole with acyl chloride in the presence of AlCl3, and demethylation over AlCl3 at 60° for 7 h gave a solid containing 99.5% I [R1 = 5-NO2, R = n-Bu] after purification Heating 3-(1-hydroxypentylidene)-5-nitro-2(3H)- benzofuran in the presence of acetic anhydride/H2SO4 for 2 h gave acid II (m.p. = 207°). 141627-42-19, 2-(n-Buty1)-3-(4-methoxybenzoy1)-5-nitrobenzofuranΤТ

856758-02-6P, 2-(n-Butyl)-3-carboxy-5-nitrobenzofuran

^{*} STRUCTURE DIAGRAM TOO LARGE FOR DISPLAY - AVAILABLE VIA OFFLINE PRINT *

RN 856758-02-6 CAPLUS
CN 3-Benzofurancarboxylic acid, 2-butyl-5-nitro- (CA INDEX NAME)

NAME)

RN 856758-03-7 CAPLUS CN 3-Benzofurancarbonyl chloride, 2-butyl-5-nitro- (CA INDEX NAME)

$$O_2N \longrightarrow \bigcup_{b} O_{ab}$$

RN 856758-04-8 CAPLUS
CN Methanone, (2-butyl-5-nitro-3-benzofuranyl)(2-methoxyphenyl)- (CA INDEX NAME)

IT 856758-05-9P, 2-(n-Butyl)-3-(2-hydroxybenzoyl)-5-nitrobenzofuran RL: BYP (Byproduct); IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent) (process for preparation de 2-(n-alkyl)-3-(4-hydroxybenzoyl)benzofurans and

intermediates by halogenation of the corresponding carboxybenzofurans, Friedel-Crafts acylation with alkoxybenzenes and dealkylation)

RN 856758-05-9 CAPLUS

CN Methanone, (2-butyl-5-nitro-3-benzofuranyl)(2-hydroxyphenyl)- (CA INDEX NAME)

IT 349102-73-4, 3-(1-Hydroxypentylidene)-5-nitro-2(3H)-benzofuranone RL: RCT (Reactant); RACT (Reactant or reagent)

(process for preparation de 2-(n-alkyl)-3-(4-hydroxybenzoyl) benzofurans and intermediates by halogenation of the corresponding carboxybenzofurans, Friedel-Crafts acylation with alkoxybenzenes and dealkylation)

RN 349102-73-4 CAPLUS

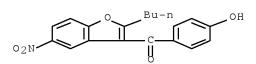
CN 2(3H)-Benzofuranone, 3-(1-hydroxypentylidene)-5-nitro- (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ & & \\ \end{array}$$

(product; process for preparation de 2-(n-alkyl)-3-(4-hydroxybenzoyl)benzofurans and intermediates by halogenation of the corresponding carboxybenzofurans, Friedel-Crafts acylation with alkoxybenzenes and dealkylation)

RN 141645-16-1 CAPLUS

CN Methanone, (2-butyl-5-nitro-3-benzofuranyl)(4-hydroxyphenyl)- (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L24 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2001:524688 CAPLUS Full-text

DOCUMENT NUMBER: 135:92535

TITLE: Process for the preparation of

3-(1-hydroxypentylidene)-5-nitro-3H-benzofuran-2-one

and its ketone tautomeric form

3-(1-oxo-pentyl)-5-nitro-3H-benzofuran-2-one

INVENTOR(S): Schouteeten, Alain; Mordacq,

Francoise

PATENT ASSIGNEE(S): Clariant (France) S.A., Fr.

SOURCE: Eur. Pat. Appl., 5 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PA: | PATENT NO. | | | | |) | DATE | | | APE | PLICAT | CION | NO. | | D | ATE | |
|---------|----------------------|------|-----------------|-----|----------------|---|-------|----------------------|-----|-----|----------------|-------|------|-----|-----|----------------------|-----|
| EP | 1116 1116 1116 | 719 | | | A2 A3 B1 | | 2001 | 0718 1024 0406 | | EP | 2001- | -8100 | 33 | | 2 | 0010 | 115 |
| D.F. | | AT, | BE, | CH, | | | , ES, | | GB, | GF | R, IT, | LI, | LU, | NL, | SE, | MC, | PT, |
| | 2803 2803 | 846 | · | · | A1 B1 | | 2001 | 0720 0405 | : | FR | 2000- | -523 | | | 2 | 0000 | 117 |
| TW | 5642 2001 | 46 | | | B A2 | | 2003 | 1201 0128 | | | 2001- | | 0495 | | | 0010 0010 | |
| AT | 2926 2238 | 30 | 10 | | T | | 2005 | 0415 | i | ΑT | 2001- | -8100 | | | 2 | 0010 0010 | 115 |
| NO | 2001 | 0002 | 65 | | A A | | 2001 | 0718 0828 | 1 | ИО | 2001- | -265 | | | 2 | 0010 0010 0010 | 116 |
| KR | 7885 1306 | 29 | | | В1 | | 2007 | 1224 | | KR | 2001-2001- | -2333 | | | 2 | 0010 0010 0010 | 116 |
| CN | 1204 | 133 | | | С | | 2005 | 0601 | | | 2001- | | | | | 0010 | |
| US | 6515 2003 | 147 | | | В2 | | 2003 | 0204 | | | 2003- | | | | | 0030 | |
| | 3975 | 5 | | | E1 | | | 0731 | 1 | US | 2005- 2000- | -5062 | 7 | | 2 | 0050 0050 0000 | 203 |
| INIONII | | | 11 4 1 O | | | | | | 1 | | 2001- | | | | | 0010 | |

OTHER SOURCE(S): CASREACT 135:92535

AB 3-(1-Hydroxypentylidene)-5-nitro-3H-benzofuran-2-one, and to its ketone tautomeric form 3-(1-oxo-pentyl)-5-nitro-3H-benzofuran-2-one, are prepared in high yield and selectivity by the reaction of 5-nitro-3H-benzofuran-2-one at >30° with pentanoic anhydride and a salt of pentanoic acid, optionally in the presence of pentanoic acid, then the resulting reaction mixture is acidified (e.g., sulfuric acid) and the precipitated product (m.p. 164°, DSC) collected by filtration.

IT 349102-73-4P 349102-74-5P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(process for the preparation of 3-(1-hydroxypentylidene)-5-nitro-3H-benzofuran-2-one and its ketone tautomeric form

3-(1-oxo-pentyl)-5-nitro-3H-benzofuran-2-one)

RN 349102-73-4 CAPLUS

CN 2(3H)-Benzofuranone, 3-(1-hydroxypentylidene)-5-nitro- (CA INDEX NAME)

RN 349102-74-5 CAPLUS CN 2(3H)-Benzofuranone, 5-nitro-3-(1-oxopentyl)- (CA INDEX NAME)

$$\circ_{2^{\mathbb{N}}} \overset{\circ}{ \underset{\mathbb{C}^{-\mathrm{Bu-n}}}{ \overset{\circ}{ =} }}$$

STRUCTURE SEARCH

=> fil reg; d stat que 116; fil capl; d que nos 118 FILE 'REGISTRY' ENTERED AT 09:53:57 ON 23 DEC 2008 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2008 American Chemical Society (ACS)

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STRUCTURE FILE UPDATES: 22 DEC 2008 HIGHEST RN 1088779-12-7 DICTIONARY FILE UPDATES: 22 DEC 2008 HIGHEST RN 1088779-12-7

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L5 STR

VAR G1=O/C VPA 10-1/2/5/6 U NODE ATTRIBUTES: CONNECT IS E1 RC AT 13 DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

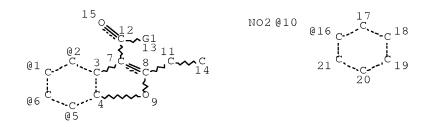
GRAPH ATTRIBUTES:
RSPEC I

NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE

L8 129 SEA FILE=REGISTRY SSS FUL L5

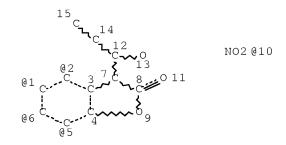
L9 STR



VAR G1=OH/X/16 VPA 10-1/2/5/6 U NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RSPEC I NUMBER OF NODES IS 21

STEREO ATTRIBUTES: NONE L11 STR



VPA 10-1/2/5/6 U
NODE ATTRIBUTES:
CONNECT IS E3 RC AT 12
CONNECT IS E1 RC AT 13
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES: RSPEC I NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE L16 57 SEA FILE=REGISTRY SUB=L8 SSS FUL (L9 OR L11)

100.0% PROCESSED 59 ITERATIONS 57 ANSWERS SEARCH TIME: 00.00.01

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FILE COVERS 1907 - 23 Dec 2008 VOL 149 ISS 26 FILE LAST UPDATED: 22 Dec 2008 (20081222/ED)

Caplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2008.

Effective October 17, 2005, revised CAS Information Use Policies apply. They are available for your review at:

http://www.cas.org/legal/infopolicy.html
'OBI' IS DEFAULT SEARCH FIELD FOR 'CAPLUS' FILE

L5 STR

L8 129 SEA FILE=REGISTRY SSS FUL L5

L9 STR

L11 STR

L16 57 SEA FILE=REGISTRY SUB=L8 SSS FUL (L9 OR L11)

L18 17 SEA FILE=CAPLUS SPE=ON ABB=ON L16

=> s 118 not 124

L25 15 L18 NOT L24 L24=INVENTOR SEARCH ANSWER SET

=> d ibib abs hitstr 125 1-15; fil hom

L25 ANSWER 1 OF 15 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2008:1399311 CAPLUS Full-text

DOCUMENT NUMBER: 149:556432

TITLE: Process for preparation of

2-(n-butyl)-3-(4-hydroxybenzoyl)-5-nitrobenzofuran

starting from 4-nitrophenol

INVENTOR(S): Diouf, Ousmanne; Durand, Thierry; Lemeune, Stephane;

Marcoux, Jean-Francois; Frison, Natacha; Larquetoux,

Laurent; Folleas, Benoit

PATENT ASSIGNEE(S): Finorga, Fr.

SOURCE: PCT Int. Appl., 9pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: French

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

| PATENT NO. | | | KIN | D | DATE | | | APPL | ICAT | I NOI | . O <i>l</i> | | D. | ATE | |
|------------|-------|-----|-----|-----|------|------|-----|------|------|-------|--------------|-----|-----|------|-----|
| | | | | _ | | | | | | | | | _ | | |
| WO 2008139 | 057 | | A2 | | 2008 | 1120 | | WO 2 | 008- | FR47: | 2 | | 2 | 0800 | 404 |
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| CP | , СН, | CN, | CO, | CR, | CU, | CZ, | DE, | DK, | DM, | DO, | DZ, | EC, | EE, | EG, | ES, |

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              TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD,
              TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW,
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                                  20081010
                                               FR 2007-2544
                                                                         20070406
     FR 2914644
                           Α1
PRIORITY APPLN. INFO.:
                                                FR 2007-2544
                                                                     A 20070406
                           CASREACT 149:556432
OTHER SOURCE(S):
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The invention is related to a process for the preparation of 2-(n-buty1)-3-(4hydroxybenzoyl)-5-nitrobenzofuran (I), intermediate in the synthesis of cardiovascular agent dronedarone, by iodination or bromination of 4nitrophenol with NBS or NIS in aqueous media in the presence of HBF4, followed by cyclization of o-iodo or o-bromophenol through a Sonogashira reaction with 1-hexyne in the presence of a N-base, catalytic amts. of Pd(II) salts or complexes and CuI, acylation of 2-(n-butyl)-5-nitrobenzofuran with 4methoxybenzoic acid or its acid halide in the presence of a Lewis acid, and demethylation in the presence of pyridinium chloride. The invention allows preparation of I by a low polluting catalytic process in very good yields. Thus, iodination of 4-nitrophenol with NIS in MeCN in the presence of HBF4 in Et20 at -20° for 5 h, addition of Pd(PPh3)2Cl2 to a mixture containing 2-iodo-4-nitrophenol, DMF, 1-hexyne, NEt3 and CuI, heating at 65° for 36 h, acylation of 2-(n-butyl)-5-nitrobenzofuran with p-anisoyl chloride in the presence of AlC13 in DCM and demethylation of 2-(n-butyl)-3-(4-methoxybenzoyl)-5nitrobenzofuran in DCM in the presence of AlCl3 at reflux for 21 h gave I. 141645-16-1P, 2-Butyl-3-(4-hydroxybenzoyl)-5-nitrobenzofuran

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(preparation of 2-(n-buty1)-3-(4-hydroxybenzoy1)-5-nitrobenzofuran starting from 4-nitrophenol)

RN 141645-16-1 CAPLUS

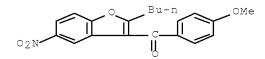
CN Methanone, (2-butyl-5-nitro-3-benzofuranyl)(4-hydroxyphenyl)- (CA INDEX NAME)

IT 141627-42-1P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of 2-(n-butyl)-3-(4-hydroxybenzoyl)-5-nitrobenzofuran via acylation with 4-methoxybenzoic acid)

RN 141627-42-1 CAPLUS

CN Methanone, (2-butyl-5-nitro-3-benzofuranyl)(4-methoxyphenyl)- (CA INDEX NAME)



L25 ANSWER 2 OF 15 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2008:1219885 CAPLUS <u>Full-text</u>

DOCUMENT NUMBER: 149:448197

TITLE: Process for preparation of

2-(n-butyl)-3-(4-hydroxybenzoyl)-5-nitrobenzofuran

starting from 4-nitrophenol

INVENTOR(S): Diouf, Ousmanne; Durand, Thierry; Lemeune, Stephane;

Marcoux, Jean Francois; Frison, Natacha; Larquetoux,

Laurent; Folleas, Benoit

PATENT ASSIGNEE(S): Finorga, Fr.

SOURCE: Fr. Demande, 13pp.

CODEN: FRXXBL

DOCUMENT TYPE: Patent LANGUAGE: French

FAMILY ACC. NUM. COUNT: 2

PATENT INFORMATION:

| PA' | TENT | NO. | | | KIN: | D | DATE | | 1 | APPL | ICAT | ION 1 | NO. | | D | ATE | |
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| FR | 2914 | 644 | | | A1 | _ | 2008 | 1010 | - | FR 2 | 007- | 2544 | | | | 0070 | |
| WO | 2008 | 1390 | 57 | | A2 | | 2008 | 1120 | 1 | WO 2 | 008- | FR47. | 2 | | 2 | 0080 | 404 |
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| | | ME, | MG, | MK, | MN, | MW, | MX, | MY, | MZ, | NA, | NG, | NΙ, | NO, | NZ, | OM, | PG, | PH, |
| | | PL, | PT, | RO, | RS, | RU, | SC, | SD, | SE, | SG, | SK, | SL, | SM, | SV, | SY, | ΤJ, | TM, |
| | | TN, | TR, | TT, | TZ, | UA, | UG, | US, | UZ, | VC, | VN, | ZA, | ZM, | ZW | | | |
| | RW: | ΑT, | BE, | ВG, | CH, | CY, | CZ, | DE, | DK, | EE, | ES, | FI, | FR, | GB, | GR, | HR, | HU, |
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| | | TR, | BF, | ВJ, | CF, | CG, | CI, | CM, | GΑ, | GN, | GQ, | GW, | ML, | MR, | NE, | SN, | TD, |
| | | ΤG, | BW, | GH, | GM, | KE, | LS, | MW, | MZ, | NA, | SD, | SL, | SZ, | TZ, | UG, | ZM, | ZW, |
| | | ΑM, | AΖ, | BY, | KG, | KZ, | MD, | RU, | ТJ, | TM | | | | | | | |
| PRIORIT | Y APP | LN. | INFO | .: | | | | | | FR 2 | 007- | 2544 | | | A 2 | 0070 | 406 |

TRIORITI AFFEN, INFO.

CASREACT 149:448197 OTHER SOURCE(S): The invention is related to a process for the preparation of 2-(n-buty1)-3-(4hydroxybenzoyl)-5-nitrobenzofuran (I), intermediate in the synthesis of cardiovascular agent dronedarone, by iodination or bromination of 4nitrophenol with NBS or NIS in aqueous media in the presence of HBF4, followed by cyclization of o-iodo or o-bromophenol through a Sonogashira reaction with 1-hexyne in the presence of a N-base, catalytic amts. of Pd(II) salts or complexes and CuI, acylation of 2-(n-butyl)-5-nitrobenzofuran with 4methoxybenzoic acid or its acid halide in the presence of a Lewis acid, and demethylation in the presence of pyridinium chloride. The invention allows preparation of I by a low polluting catalytic process in very good yields. Thus, iodination of 4-nitrophenol with NIS in MeCN in the presence of HBF4 in Et20 at -20° for 5 h, addition of Pd(PPh3)2Cl2 to a mixture containing 2-iodo-4-nitrophenol, DMF, 1-hexyne, NEt3 and CuI, heating at 65° for 36 h, acylation of 2-(n-butyl)-5-nitrobenzofuran with p-anisoyl chloride in the presence of AlCl3 in DCM and demethylation of 2-(n-butyl)-3-(4-methoxybenzoyl)-5nitrobenzofuran in DCM in the presence of AlCl3 at reflux for 21 h gave I.

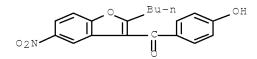
IT 141645-16-1P, 2-Butyl-3-(4-hydroxybenzoyl)-5-nitrobenzofuran

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(preparation of 2-(n-butyl)-3-(4-hydroxybenzoyl)-5-nitrobenzofuran starting from <math>4-nitrophenol)

RN 141645-16-1 CAPLUS

CN Methanone, (2-butyl-5-nitro-3-benzofuranyl)(4-hydroxyphenyl)- (CA INDEX NAME)



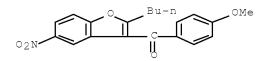
IT 141627-42-1P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of 2-(n-buty1)-3-(4-hydroxybenzoy1)-5-nitrobenzofuran via acylation with 4-methoxybenzoic acid)

RN 141627-42-1 CAPLUS

CN Methanone, (2-butyl-5-nitro-3-benzofuranyl)(4-methoxyphenyl)- (CA INDEX NAME)



REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 3 OF 15 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2007:1420616 CAPLUS Full-text

DOCUMENT NUMBER: 148:54878

TITLE: Process for preparation of

2-butyl-3-(4-methoxybenzoyl)-5-nitrobenzofuran by

reaction of 2-butyl-5-nitrobenzofuran using non-halogenated solvents in the reaction and/or $\,$

extraction steps.

INVENTOR(S):
Eklund, Lars

PATENT ASSIGNEE(S): Cambrex Karlskoga AB, Swed.

SOURCE: PCT Int. Appl., 16pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATEN | IT NO. | | | KIN | D | DATE | | | APPL | ICAT | ION I | NO. | | D | ATE | |
|-------|--------|-----|-----|-----|-----|------|------|-----|------|-------|-------|-----|-----|-----|------|-----|
| | | | | | _ | | | | | | | | | | | |
| WO 20 | 071409 | 89 | | A2 | | 2007 | 1213 | | WO 2 | 007-1 | EP49 | 84 | | 2 | 0070 | 605 |
| WO 20 | 071409 | 89 | | АЗ | | 2008 | 0717 | | | | | | | | | |
| W | : AE, | AG, | AL, | AM, | ΑT, | ΑU, | ΑZ, | BA, | BB, | BG, | BH, | BR, | BW, | BY, | BZ, | CA, |
| | CH, | CN, | CO, | CR, | CU, | CZ, | DE, | DK, | DM, | DO, | DZ, | EC, | EE, | EG, | ES, | FΙ, |

GB, GD, GE, GH, GM, GT, HN, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR, KZ, LA, LC, LK, LR, LS, LT, LU, LY, MA, MD, MG, MK, MN, MW, MX, MY, MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RS, RU, SC, SD, SE, SG, SK, SL, SM, SV, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, ZA, ZM, ZW

RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, LV, MC, MT, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ,

BY, KG, KZ, MD, RU, TJ, TM, AP, EA, EP, OA

PRIORITY APPLN. INFO.: GB 2006-11210 A 20060607

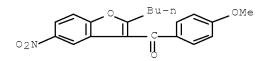
OTHER SOURCE(S): CASREACT 148:54878

AB A process for the production of 2-butyl-3-(4-methoxybenzoyl)-5-nitrobenzofuran by reaction of 2-butyl-5-nitrobenzofuran uses non-halogenated solvents in the reaction and/or extraction by crystallization of the product. Thus, reaction of 2-butyl-5-nitrobenzofuran with 4-methoxybenzoyl chloride in o-nitrotoluene in the presence of FeCl3 gave 82% 2-butyl-3-(4-methoxybenzoyl)-5-nitrobenzofuran.

IT 141627-42-1P, 2-Butyl-3-(4-methoxybenzoyl)-5-nitrobenzofuran RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (preparation of butylmethoxybenzoylnitrobenzofuran by reaction of butylnitrobenzofuran using non-halogenated solvents in the reaction and/or extraction steps)

RN 141627-42-1 CAPLUS

CN Methanone, (2-butyl-5-nitro-3-benzofuranyl)(4-methoxyphenyl)- (CA INDEX NAME)



L25 ANSWER 4 OF 15 CAPLUS COPYRIGHT 2008 ACS on STN

ACCESSION NUMBER: 2006:409442 CAPLUS <u>Full-text</u>

DOCUMENT NUMBER: 144:450603

TITLE: Process for acylation of (hydroxy)-containing aromatic

compounds, particularly benzothiophenes, with aromatic hydroxycarboxylic acids in the presence of Lewis acids

and halogenosilanes

INVENTOR(S): Bourgeois, Damien
PATENT ASSIGNEE(S): Rhodia Chimie, Fr.
SOURCE: Fr. Demande, 35 pp.

CODEN: FRXXBL

DOCUMENT TYPE: Patent LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|----------------|---------|-------------|---------------------|-----------------|
| | | | | |
| FR 2877341 | A1 | 20060505 | FR 2004-11646 | 20041102 |
| CA 2585714 | A1 | 20060511 | CA 2005-2585714 | 20051028 |
| WO 2006048545 | A1 | 20060511 | WO 2005-FR2716 | 20051028 |
| W: AE, AG, AL, | AM, AT, | , AU, AZ, E | BA, BB, BG, BR, BW, | BY, BZ, CA, CH, |
| CN, CO, CR, | CU, CZ, | , DE, DK, I | DM, DZ, EC, EE, EG, | ES, FI, GB, GD, |

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GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KM, KN, KP, KR,
             KZ, LC, LK, LR, LS, LT, LU, LV, LY, MA, MD, MG, MK, MN, MW, MX,
             MZ, NA, NG, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE,
             SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC,
             VN, YU, ZA, ZM, ZW
         RW: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE,
             IS, IT, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ,
             CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG, BW, GH,
             GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY,
             KG, KZ, MD, RU, TJ, TM
     EP 1809617
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             IS, IT, LI, LT, LU, LV, MC, NL, PL, PT, RO, SE, SI, SK, TR
     IN 2007DN03286
                                20070831
                                            IN 2007-DN3286
                                                                    20070501
                          Α
     US 20080154049
                                20080626
                                            US 2008-666877
                                                                    20080214
                          Α1
PRIORITY APPLN. INFO.:
                                            FR 2004-11646
                                                                A 20041102
                                            WO 2005-FR2716
                                                                W
                                                                   20051028
OTHER SOURCE(S):
                        CASREACT 144:450603; MARPAT 144:450603
GΙ
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$$[R^5]_n$$
 $[R^7]_m$
 $[R^7]_m$
 $[R^7]_m$
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 $[R^7]_m$
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 $[R^7]_m$

The invention is related to a process for the acylation of aromatic compds., particularly benzothiophenes I [R4 = alkyl, halogenophenyl, (un)substituted Ph; each R5 = independently H, NO2, alkyl, alkoxy, halo, CF3, etc.; n = 0-3], with aromatic hydroxycarboxylic acids II [each R7 = H or a substituent, especially alkyl, alkoxy, NO2, CN; m < 4], in the presence of a Lewis acid and a halogenosilane to give the ketones III. The advantages include acylation of hydroxy-containing substrates and/or agents without OH group protection, absence of toxic materials and simple procedure. Thus, successive addition of 4-hydroxybenzoic acid, chlorobenzene, methyltrichlorosilane, 2-butyl-5-nitrobenzofuran (IV) and FeCl3 at 23°, and stirring at 40° for 5 h gave 2-butyl-3-(4-hydroxybenzoyl)-5-nitrobenzofuran in 78% selectivity at 95% conversion of IV.

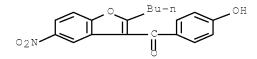
IT 141645-16-1P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(ketone product; process for acylation of aromatic compds., particularly benzothiophenes with carboxylic acids, especially aryl hydroxycarboxylic acids in presence of Lewis acids and halogenosilanes)

RN 141645-16-1 CAPLUS

CN Methanone, (2-butyl-5-nitro-3-benzofuranyl)(4-hydroxyphenyl)- (CA INDEX NAME)



REFERENCE COUNT: 9 THERE ARE 9 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 5 OF 15 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2002:975672 CAPLUS <u>Full-text</u>

DOCUMENT NUMBER: 138:24636

TITLE: Preparation of 2-alkyl-3-acylbenzofurans from O-aryl

oximes

INVENTOR(S): Kano, Hitoshi; Kogami, Kenji; Iida, Yukio PATENT ASSIGNEE(S): Sumitomo Seika Chemicals Co., Ltd., Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 7 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|--------|--------------|--------------------|----------|
| | | | | |
| JP 2002371076 | A | 20021226 | JP 2001-179457 | 20010614 |
| PRIORITY APPLN. INFO.: | | | JP 2001-179457 | 20010614 |
| OTHER COHROLICA | CACDEA | CT 120.24626 | . MADDAT 120.2/626 | |

OTHER SOURCE(S): CASREACT 138:24636; MARPAT 138:24636

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$$\begin{array}{c|c} R^2 & & \\$$

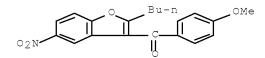
- Title compds. I (R1 = alkyl; R2 = H, halo, cyano, nitro, formyl, alkyl, alkylcarbonyl, alkoxy, alkoxycarbonyl; R3 = alkyl, Ph, substituted Ph) are prepared by cyclization of R2C6H4ON:CR1Me in the presence of acids followed by acylation with R3COCl in the presence of Lewis acids. Thus, cyclization of O- (4-nitrophenyl)-2-butanone in EtOH the presence of H2SO4 gave, after treatment with 4-nitrobenzoyl chloride in the presence of SnC14, 70.8% 2-ethyl-3-(4-nitrobenzoyl)-5-nitrobenzofuran.
- IT 141627-42-1P 141645-23-0P 478158-83-7P

RL: IMF (Industrial manufacture); SPN (Synthetic preparation); PREP (Preparation)

(preparation of 2-alkyl-3-acylbenzofurans from 0-aryl oximes by cyclization and acylation)

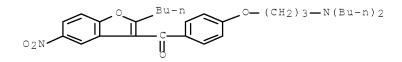
RN 141627-42-1 CAPLUS

CN Methanone, (2-butyl-5-nitro-3-benzofuranyl)(4-methoxyphenyl)- (CA INDEX NAME)



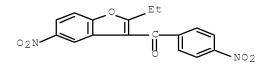
RN 141645-23-0 CAPLUS

CN Methanone, (2-butyl-5-nitro-3-benzofuranyl)[4-[3-(dibutylamino)propoxy]phenyl]- (CA INDEX NAME)



RN 478158-83-7 CAPLUS

Methanone, (2-ethyl-5-nitro-3-benzofuranyl)(4-nitrophenyl)- (CA INDEX CN



L25 ANSWER 6 OF 15 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2002:465950 CAPLUS Full-text

DOCUMENT NUMBER: 137:33204

TITLE: 2-Butyl-3-(4-[3-(dibutylamino)propoxy]benzoyl)-5-nitro-

benzofuran hydrochloride and preparation thereof

INVENTOR(S): Biard, Michel

PATENT ASSIGNEE(S): Sanofi-Synthelabo, Fr. SOURCE: PCT Int. Appl., 25 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: French

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| PATENT | NO. | | | KIN | D | DATE | | APPLICATION NO. | | | | | | D | ATE | |
|---------|------|--------|-----|-----|-----|------|------|-----------------|------|------|------|-----|-----|-----|------|-----|
| WO 2002 | 0480 | 78 | | A1 | _ | 2002 | 0620 | , | | | | | | 2 | 0011 | 210 |
| W: | ΑE, | AG, | AL, | AM, | ΑT, | AU, | AZ, | BA, | BB, | BG, | BR, | BY, | BZ, | CA, | CH, | CN, |
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| | GM, | HR, | HU, | ID, | IL, | IN, | IS, | JP, | ΚE, | KG, | KP, | KR, | KΖ, | LC, | LK, | LR, |
| | LS, | LT, | LU, | LV, | MA, | MD, | MG, | MK, | MN, | MW, | MX, | MZ, | NO, | NZ, | OM, | PH, |
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| | UA, | UG, | US, | UZ, | VN, | YU, | ZA, | ZM, | ZW | | | | | | | |
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| | CY, | DE, | DK, | ES, | FI, | FR, | GB, | GR, | ΙE, | ΙΤ, | LU, | MC, | NL, | PT, | SE, | TR, |
| | BF, | ВJ, | CF, | CG, | CI, | CM, | GA, | GN, | GQ, | GW, | ML, | MR, | NE, | SN, | TD, | ΤG |
| FR 2817 | 865 | | | A1 | | 2002 | 0614 | | FR 2 | 000- | 1606 | 9 | | 2 | 0001 | 211 |

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FR 2817865
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                                 20040527
                                             JP 2002-549615
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     HU 2005000981
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     IN 2008DN01265
                                 20080425
                                             IN 2008-DN1265
                                                                     20080213
                           Α
PRIORITY APPLN. INFO.:
                                             FR 2000-16069
                                                                  A 20001211
                                             WO 2001-FR3900
                                                                  W 20011210
                                             IN 2003-DN816
                                                                  A3 20030526
OTHER SOURCE(S):
                         CASREACT 137:33204; MARPAT 137:33204
GΙ
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AB A process for the synthesis of 2-butyl-3-(4-[3-(dibutylamino)propoxy]benzoyl)-5-nitro-benzofuran (I) hydrochloride and use of I in the synthesis of dronedarone hydrochloride were disclosed. 4-[3-(Dibutylamino)propoxy]benzoyl chloride was used to acylate 2-butyl-5-nitrobenzofuran (C6H5Cl, FeCl3, $0^{\circ}\rightarrow22^{\circ}\text{C}$, 1.5 h) to give title compound I after neutralization of the hydrochloride salt. Reduction of I (EtOH, 3.4 atm H2, PtO, 20 min) followed by treatment with MsCl/Et3N in CH2Cl2 provided dronedarone. Compared to prior art, the current method avoids the environmental burden of excessive use of aluminum chloride in the acylation step.

IT 141645-23-0P 437651-47-3P

RL: IMF (Industrial manufacture); RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent) (intermediate; process for the synthesis of 2-(butyl)-3-(4-[3-(dibutylamino)propoxy]benzoyl)-5-nitro-benzofuran hydrochloride and conversion to dronedarone)

RN 141645-23-0 CAPLUS

CN Methanone, (2-butyl-5-nitro-3-benzofuranyl) [4-[3-(dibutylamino)propoxy]phenyl]- (CA INDEX NAME)

RN 437651-47-3 CAPLUS

Methanone, (2-butyl-5-nitro-3-benzofuranyl)[4-[3-CN (dibutylamino)propoxy]phenyl]-, hydrochloride (1:1) (CA INDEX NAME)

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THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS REFERENCE COUNT: 2 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 7 OF 15 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2000:700546 CAPLUS Full-text

DOCUMENT NUMBER: 134:4829

TITLE: Synthesis of 2-dimethylamino-3-hetaryl-5-

hydroxybenzofurans by the Nenitzescu route from nitro-containing enamines of the benzofuran series Mukhanova, T. I.; Alekseeva, L. M.; Granik, V. G.

CORPORATE SOURCE: The State Science Center of the Russian Federation

"NIOPIK", Moscow, 103787, Russia

SOURCE: Chemistry of Heterocyclic Compounds (New

York) (Translation of Khimiya Geterotsiklicheskikh

Soedinenii) (2000), 36(4), 410-415 CODEN: CHCCAL; ISSN: 0009-3122

PUBLISHER: Consultants Bureau

DOCUMENT TYPE: Journal LANGUAGE: English

OTHER SOURCE(S): CASREACT 134:4829

Enamines of the benzofuran series which contain nitro groups in the benzene ring of benzofuran or in 3-benzoyl substituent react with benzoquinone to form 2-dimethylamino-3-(substituted benzo-2-furyl)-5-hydroxybenzofurans.

308796-99-8P 308797-00-4P 308797-01-5P ΙT

308797-03-7P

AUTHOR(S):

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of 2-dimethylamino-3-hetaryl-5-hydroxybenzofurans by the Nenitzescu route from nitro-containing enamines of the benzofuran series)

308796-99-8 CAPLUS RN

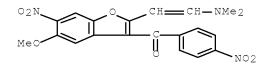
CN Methanone, [2-[2-(dimethylamino)ethenyl]-5-methoxy-6-nitro-3benzofuranyl]phenyl- (CA INDEX NAME)

RN 308797-00-4 CAPLUS

CN Methanone, [2-[2-(dimethylamino)ethenyl]-5-methoxy-6-nitro-3-benzofuranyl](4-methylphenyl)- (CA INDEX NAME)

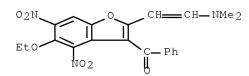
RN 308797-01-5 CAPLUS

CN Methanone, [2-[2-(dimethylamino)ethenyl]-5-methoxy-6-nitro-3-benzofuranyl](4-nitrophenyl)- (CA INDEX NAME)



RN 308797-03-7 CAPLUS

CN Methanone, [2-[2-(dimethylamino)ethenyl]-5-ethoxy-4,6-dinitro-3-benzofuranyl]phenyl- (CA INDEX NAME)



REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L25 ANSWER 8 OF 15 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1996:393883 CAPLUS Full-text

DOCUMENT NUMBER: 125:58304

ORIGINAL REFERENCE NO.: 125:11205a,11208a

TITLE: Preparation of 3-benzoylbenzofurans as thyroid hormone

antagonists

INVENTOR(S): Mellin, Charlotta
PATENT ASSIGNEE(S): Karo Bio Ab, Swed.
SOURCE: PCT Int. Appl., 79 pp.

CODEN: PIXXD2

DOCUMENT TYPE: Patent LANGUAGE: English

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PA | PATENT NO. | | | KINI |) | DATE | | I | APP | LICAT | ION | NO. | | D | ATE | | |
|---------|-------------------|------|-----|-----------|-----|---------|-----|-----|--------|-------|------|-----|-----|-----|-------|-----|----|
| WC | 9605190 W: AU, | CA, | | A1 KR, | | 19960 | 222 | V | WO | 1995- | EP32 | 14 | | 1 | 9950 | 311 | |
| | RW: AT, | BE, | CH, | DE, | DK | , ES, I | FR, | GB, | GR | , IE, | ΙΤ, | LU, | MC, | NL, | PT, | SE | |
| CA | 2197185 | | | A1 | | 19960 | 222 | | CA | 1995- | 2197 | 185 | | 1 | 99508 | 311 | |
| AU | 9533455 | | | Α | | 19960 | 307 | I | UA | 1995- | 3345 | 5 | | 1 | 99508 | 311 | |
| AU | 694551 | | | В2 | | 19980 | 723 | | | | | | | | | | |
| EP | 775129 | | | A1 | | 19970. | 528 | E | ΞP | 1995- | 9298 | 66 | | 1 | 99508 | 311 | |
| EP | 775129 | | | В1 | | 19981 | 021 | | | | | | | | | | |
| | R: AT, | BE, | CH, | DE, | DK, | ES, | FR, | GB, | GR | , IE, | ΙΤ, | LI, | LU, | MC, | NL, | PT, | SE |
| JP | 10504297 | , | | T | | 19980 | 428 | | JΡ | 1995- | 5070 | 25 | | 1 | 99508 | 311 | |
| AT | 172460 | | | Τ | | 19981 | 115 | I | TA | 1995- | 9298 | 66 | | 1 | 9950 | 311 | |
| ES | 2123287 | | | Т3 | | 19990 | 101 | E | ΞS | 1995- | 9298 | 66 | | 1 | 9950 | 311 | |
| US | 5854282 | | | Α | | 19981 | 229 | J | JS | 1997- | 7769 | 24 | | 1 | 9970 | 107 | |
| PRIORIT | Y APPLN. | INFO | .: | | | | | | GΒ | 1994- | 1621 | 9 | | A 1 | 99408 | 311 | |
| | | | | | | | | V | ΝO | 1995- | EP32 | 14 | | W 1 | 99508 | 311 | |

OTHER SOURCE(S): MARPAT 125:58304

GΙ

AB Title compds. (I; R = CH2CO2H; R1 = alkyl; R2 = NHSO2R3, NHCOR3, NHCONHR3; R3 = CF3, alkyl, C6H4R4-4; R4 = OH, F, alkoxy, NO2; R5 = Br or iodo; Z = CH2 or CO) were prepared Thus, the Wittig reagent prepared from 2-hydroxy-5-nitrobenzyl bromide was cyclocondensed with BuCOCl and the product acylated with 4-(MeO)C6H4COCl to give I (R = Me, R1 = Bu, R2 = NO2, R5 = H, Z = CO) which was converted in 5 steps to title compound II. Data for inhibition by I of triiodothyronine-induced expression of alkaline phosphatase by thyroid hormone reporter cells were given in graphic form.

IT 141627-42-1P 141627-44-3P 141645-16-1P 141645-18-3P 178239-69-5P 178239-70-8P

178239-81-1P 178239-82-2P 178239-88-8P

178239-89-9P 178239-93-5P 178239-94-6P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation of 3-benzoylbenzofurans as thyroid hormone antagonists)

RN 141627-42-1 CAPLUS

CN Methanone, (2-butyl-5-nitro-3-benzofuranyl)(4-methoxyphenyl)- (CA INDEX NAME)

$$\circ_2 \mathbb{N} \qquad \stackrel{\circ}{\longrightarrow} \stackrel{\mathbb{B}u-n}{\longleftarrow} \circ_{\mathbb{M}^{\epsilon}}$$

RN 141627-44-3 CAPLUS

CN Methanone, (4-methoxyphenyl)[2-(1-methylethyl)-5-nitro-3-benzofuranyl]-(CA INDEX NAME)

RN 141645-16-1 CAPLUS

CN Methanone, (2-butyl-5-nitro-3-benzofuranyl)(4-hydroxyphenyl)- (CA INDEX NAME)

RN 141645-18-3 CAPLUS

CN Methanone, (4-hydroxyphenyl)[2-(1-methylethyl)-5-nitro-3-benzofuranyl]- (CA INDEX NAME)

RN 178239-69-5 CAPLUS

CN Methanone, (2-butyl-5-nitro-3-benzofuranyl)(4-hydroxy-3,5-diiodophenyl)- (CA INDEX NAME)

RN 178239-70-8 CAPLUS

CN Acetic acid, 2-[4-[(2-butyl-5-nitro-3-benzofuranyl)carbonyl]-2,6-diiodophenoxy]-, ethyl ester (CA INDEX NAME)

$$O_2\mathbb{N} \xrightarrow{O_1} C_1 \xrightarrow{Bu-n} I$$

$$O_2\mathbb{N} \xrightarrow{O_1} C_1 \xrightarrow{C_1} C_2 = C_1$$

RN 178239-81-1 CAPLUS

CN Methanone, (4-hydroxy-3,5-diiodophenyl)[2-(1-methylethyl)-5-nitro-3-benzofuranyl]- (CA INDEX NAME)

RN 178239-82-2 CAPLUS

CN Acetic acid, 2-[2,6-diiodo-4-[[2-(1-methylethyl)-5-nitro-3-benzofuranyl]carbonyl]phenoxy]- (CA INDEX NAME)

RN 178239-88-8 CAPLUS

CN Methanone, (2-butyl-5-nitro-3-benzofuranyl)(3,5-dibromo-4-hydroxyphenyl)- (CA INDEX NAME)

RN 178239-89-9 CAPLUS

CN Acetic acid, 2-[2,6-dibromo-4-[(2-butyl-5-nitro-3-benzofuranyl)carbonyl]phenoxy]-, ethyl ester (CA INDEX NAME)

$$O_{2N} \xrightarrow{O \longrightarrow Bu-n} Br$$

$$O \longrightarrow CH2 \longrightarrow C-OEt$$

RN 178239-93-5 CAPLUS

CN Methanone, (3,5-dibromo-4-hydroxyphenyl)[2-(1-methylethyl)-5-nitro-3-benzofuranyl]- (CA INDEX NAME)

RN 178239-94-6 CAPLUS

CN Acetic acid, 2-[2,6-dibromo-4-[[2-(1-methylethyl)-5-nitro-3-benzofuranyl]carbonyl]phenoxy]-, ethyl ester (CA INDEX NAME)

L25 ANSWER 9 OF 15 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1992:426336 CAPLUS <u>Full-text</u>

DOCUMENT NUMBER: 117:26336
ORIGINAL REFERENCE NO.: 117:4747a,4750a

TITLE: Preparation of benzofurans, benzothiophenes, indoles,

and indolizines as cardiovascular agents

INVENTOR(S): Gubin, Jean; Lucchetti, Jean; Inion, Henri; Chatelain,

Pierre; Rosseels, Gilbert; Kilenyi, Steven

PATENT ASSIGNEE(S): Sanofi SA, Fr.; Societe Anon. Sanofi-Pharma N. V.

SOURCE: Eur. Pat. Appl., 81 pp.

CODEN: EPXXDW

DOCUMENT TYPE: Patent LANGUAGE: French

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | | | APPLICATION NO. | DATE |
|--|-----------|----------|-------------------------|------------|
| EP 471609 | A1 | 19920219 | EP 1991-402201 | 19910806 |
| EP 471609 | В1 | 19961127 | | |
| R: AT, BE, CH | , DE, DK | ES, FR, | GB, GR, IT, LI, LU, NL, | SE |
| FR 2665444 | A1 | 19920207 | FR 1990-10036 | 19900806 |
| FR 2665444 FR 2665444 CA 2047773 | В1 | 19921127 | | |
| CA 2047773 | A1 | 19920207 | CA 1991-2047773 | 19910724 |
| CA 2047773 | С | 20000912 | | |
| US 5223510 | A | 19930629 | | |
| ZA 9105934 | A A | 19930331 | | 19910729 |
| IL 98991 | A | 19951208 | IL 1991-98991 | 19910729 |
| AU 9181428 | A | 19920213 | AU 1991-81428 | 19910730 |
| AU 648569 | | 19940428 | | |
| FI 9103704 | A | 19920207 | FI 1991-3704 | 19910802 |
| FI 114914 | B1 | 20050131 | | |
| NO 9103033 | A | 19920207 | NO 1991-3033 | 19910805 |
| NO 179042 | В | 19960415 | | |
| NO 179042 | С | 19960724 | | |
| BR 9103354 | A | 19920505 | BR 1991-3354 | 19910805 |
| JP 04316554 | A | 19921106 | JP 1991-195431 | 19910805 |
| JP 2795759 | В2 | 19980910 | | |
| PL 168044 | | 19951230 | | |
| RU 2095357 | C1 | 19971110 | RU 1991-5001351 | 19910805 |
| CZ 288527 | В6 | 20010711 | CZ 1991-2427 | 19910805 |
| SK 283527 | В6 | 20030911 | SK 1991-2427 | 19910805 |
| HU 62280 | A2 | 19930428 | | 19910806 |
| HU 218271 | В | 20000728 | | |
| AT 145645 | T | 19961215 | | |
| HU 218271 AT 145645 ES 2096639 | Т3 | 19970316 | ES 1991-402201 | 19910806 |
| KR 190673 | B1 | | | |
| RIORITY APPLN. INFO.: | | | FR 1990-10036 | A 19900806 |
| | | | CS 1991-2427 | A 19910805 |
| TITED COLLDON (C) | 117 00 00 | 117 0000 | - | |

OTHER SOURCE(S): MARPAT 117:26336

GI

$$\mathbb{R}^{1}\mathbf{Y} = \mathbb{R}^{1}\mathbf{X} + \mathbb{R}^{2}\mathbf{X}$$

$$\mathbb{R}^{1}\mathbf{X} = \mathbb{R}^{1}\mathbf{X} + \mathbb{R}^{2}\mathbf{X}$$

AB Title compds. I [R1 = various (un)substituted benzofuryl, benzothienyl, indolyl, and indolizinyl groups; Y = CO, CH(OR4); R2 = H, alkyl; R3 = alkyl,

certain (hetero)aryl and (hetero)aralkyl; or R2R3 = alkylene or alkenylene optionally substituted by Ph or interrupted by O, NH, alkyl- or phenylimino, or N; R4 = H, alkyl, acyl; A = O, S, NHCO; when W = W' = CH or N, Z = O or S; or W, W', and Z form (un)substituted benzene nucleus; n = 1-5] were prepared For example, 2-butyl-5-nitrobenzofuran (preparation given) underwent Friedel-Crafts reaction with anisoyl chloride and SnCl4 to give 83.5% 3-(4-methoxybenzoyl) derivative, which was subjected to demethylation by AlCl3 (90.1%), etherification with Cl(CH2)3NBu2 (88.76%), hydrogenation of the NO2 group (95.28%), and N-methanesulfonylation (61.1%) to give title compound II, isolated as the HCl salt. At 10 mg/kg in anesthetized rats, II increased the duration of action potential by 60%. A formulation, 35 syntheses of I, approx. 100 addnl. listed I, addnl. action potential data, and antiadrenergic data for some I, are given. I are also said to be useful as potentiators of anticancer agents.

IT 90908-76-2P 98873-72-4P 141627-42-1P 141627-44-3P 141645-10-5P 141645-16-1P 141645-18-3P 141645-20-7P 141645-23-0P 141645-26-3P 141645-27-4P 141645-28-5P 141645-29-6P 141645-34-3P 141645-36-5P 141645-37-6P 141645-38-7P 141645-39-8P

141645-37-6P 141645-38-7P 141645-39-8P 141645-41-2P 141645-45-6P 141645-46-7P 141645-48-9P 141645-50-3P 141671-41-2P

141671-42-3P

RN

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, in preparation of cardiovascular agents) 90908-76-2 CAPLUS

CN Methanone, (2-ethyl-5-nitro-3-benzofuranyl)(4-methoxyphenyl)- (CA INDEX NAME)

RN 98873-72-4 CAPLUS

CN Methanone, (2-ethyl-5-nitro-3-benzofuranyl)(4-hydroxyphenyl)- (CA INDEX NAME)

RN 141627-42-1 CAPLUS

CN Methanone, (2-butyl-5-nitro-3-benzofuranyl)(4-methoxyphenyl)- (CA INDEX NAME)

$$\circ_2 \mathbb{N} \qquad \qquad \circ \mathbb{N} \qquad \circ \mathbb{N}$$

RN 141627-44-3 CAPLUS

CN Methanone, (4-methoxyphenyl)[2-(1-methylethyl)-5-nitro-3-benzofuranyl]- (CA INDEX NAME)

RN 141645-10-5 CAPLUS

CN Methanone, (4-methoxyphenyl)(5-nitro-2-propyl-3-benzofuranyl)- (CA INDEX NAME)

RN 141645-16-1 CAPLUS

CN Methanone, (2-butyl-5-nitro-3-benzofuranyl)(4-hydroxyphenyl)- (CA INDEX NAME)

RN 141645-18-3 CAPLUS

CN Methanone, (4-hydroxyphenyl)[2-(1-methylethyl)-5-nitro-3-benzofuranyl]- (CA INDEX NAME)

RN 141645-20-7 CAPLUS

CN Methanone, (4-hydroxyphenyl)(5-nitro-2-propyl-3-benzofuranyl)- (CA INDEX NAME)

RN 141645-23-0 CAPLUS
CN Methanone, (2-butyl-5-nitro-3-benzofuranyl)[4-[3-(dibutylamino)propoxy]phenyl]- (CA INDEX NAME)

RN 141645-26-3 CAPLUS
CN Methanone, (2-butyl-5-nitro-3-benzofuranyl) [4-[3-[(1,1-dimethylethyl)amino]propoxy]phenyl]-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 141645-25-2 CMF C26 H32 N2 O5

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 141645-27-4 CAPLUS
CN Methanone, [4-[3-(dibutylamino)propoxy]phenyl](2-ethyl-5-nitro-3-benzofuranyl)-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 141645-28-5 CAPLUS

CN Methanone, [4-[3-(dibutylamino)propoxy]phenyl](5-nitro-2-propyl-3-benzofuranyl)- (CA INDEX NAME)

RN 141645-29-6 CAPLUS

CN Methanone, (2-butyl-5-nitro-3-benzofuranyl)[4-[3-(diethylamino)propoxy]phenyl]-, hydrochloride (1:1) (CA INDEX NAME)

HC1

RN 141645-34-3 CAPLUS

CN Methanone, [4-[3-(dibutylamino)propoxy]phenyl][2-(1-methylethyl)-5-nitro-3-benzofuranyl]- (CA INDEX NAME)

RN 141645-36-5 CAPLUS

CN Methanone, [4-(2-bromoethoxy)phenyl](2-butyl-5-nitro-3-benzofuranyl)- (CA INDEX NAME)

RN 141645-37-6 CAPLUS CN Methanone, [4-[(5-bromopentyl)oxy]phenyl](2-butyl-5-nitro-3-benzofuranyl)-(CA INDEX NAME)

RN 141645-38-7 CAPLUS

CN Methanone, [4-(3-bromopropoxy)phenyl](2-butyl-5-nitro-3-benzofuranyl)-(CA INDEX NAME)

RN 141645-39-8 CAPLUS

CN Methanone, (2-butyl-5-nitro-3-benzofuranyl)[4-[2- (dibutylamino)ethoxy]phenyl]-, hydrochloride (1:1) (CA INDEX NAME)

● HCl

RN 141645-41-2 CAPLUS

CN Methanone, (2-butyl-5-nitro-3-benzofuranyl)[4-[[5- (dibutylamino)pentyl]oxy]phenyl]-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 141645-40-1 CMF C32 H44 N2 O5

CM 2

CRN 144-62-7 CMF C2 H2 O4

RN 141645-45-6 CAPLUS

CN Propanamide, N-[4-[(2-butyl-5-nitro-3-benzofuranyl)carbonyl]phenyl]-3-chloro- (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & & \\ & & \\ & & & \\ & &$$

RN 141645-46-7 CAPLUS

CN Butanamide, N-[4-[(2-butyl-5-nitro-3-benzofuranyl)carbonyl]phenyl]-4-chloro- (CA INDEX NAME)

$$\begin{array}{c|c} & & & \\ &$$

RN 141645-48-9 CAPLUS

CN Propanamide, N-[4-[(2-buty1-5-nitro-3-benzofurany1)carbony1]pheny1]-3-(dibutylamino)-, ethanedioate (1:1) (CA INDEX NAME)

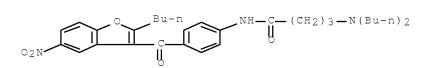
CM 1

CRN 141645-47-8 CMF C30 H39 N3 O5

RN 141645-50-3 CAPLUS
CN Butanamide, N-[4-[(2-butyl-5-nitro-3-benzofuranyl)carbonyl]phenyl]-4(dibutylamino)-, ethanedioate (1:1) (CA INDEX NAME)

CM 1

CRN 141645-49-0 CMF C31 H41 N3 O5

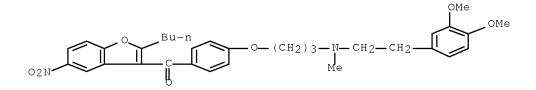


CM 2

CRN 144-62-7

CMF C2 H2 O4

CRN 141671-40-1 CMF C33 H38 N2 O7

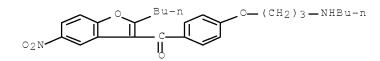


СМ 2

CRN 144-62-7 CMF C2 H2 O4

RN 141671-42-3 CAPLUS

CN Methanone, [4-[3-(butylamino)propoxy]phenyl](2-butyl-5-nitro-3benzofuranyl) - (CA INDEX NAME)



L25 ANSWER 10 OF 15 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1992:151553 CAPLUS Full-text

DOCUMENT NUMBER: 116:151553

ORIGINAL REFERENCE NO.: 116:25645a,25648a

TITLE: Preparation of benzofuran derivatives as drugs for

excretion of uric acid

Tomiyama, Takeshi; Tomiyama, Itaru; Shirai, Tadashi; INVENTOR(S):

Wakabayashi, Shuichi; Futamura, Masayuki; Ichikawa,

Senju

PATENT ASSIGNEE(S): Kotobuki Seiyaku Co., Ltd., Japan SOURCE:

Jpn. Kokai Tokkyo Koho, 11 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT:

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|--------|------------|-----------------|----------|
| | | | | |
| JP 03261778 | A | 19911121 | JP 1990-59500 | 19900309 |
| JP 2873599 | B2 | 19990324 | | |
| PRIORITY APPLN. INFO.: | | | JP 1990-59500 | 19900309 |
| OTHER SOURCE(S): | MARPAT | 116:151553 | | |
| GI | | | | |

$$\mathbb{R}^{1} \xrightarrow{\mathbb{Q}} \mathbb{R}^{2} \xrightarrow{\mathbb{R}^{3}} \mathbb{Q} \mathbb{Q} \mathbb{R}^{2} \mathbb{Q} \mathbb{Q} \mathbb{R}^{3}$$

The title derivs. I (R1 = alkyl, alkyloxy, halo, OH, etc.; R2 = alkyl; R3, R4 = H, alkyl) were prepared Reaction of 2-ethyl-6-chlorobenzofuran with 4-methoxycarbonylmethyloxy-3-methylbenzoyl chloride in CH2Cl2 containing SnCl4, followed by saponification with NaOH, acidification and workup, gave I (R1 = C1, R2 = Et, R4 = H, R3 = Me) (II). I are useful in the treatment of gout. In rats dosed with phenol red and II, the amount of phenol red in the blood is 120.9% of the amount of phenol red in controls. (The clearance of phenol red from the blood is decreased by agents promoting the excretion of uric acid.).

II 139718-02-3P

RL: RCT (Reactant); SPN (Synthetic preparation); PREP (Preparation); RACT (Reactant or reagent)

(preparation and reaction of, in preparation of drug for promoting uric

excretion)

RN 139718-02-8 CAPLUS

acid

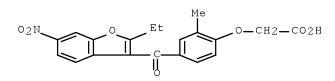
CN Acetic acid, 2-[4-[(2-ethyl-6-nitro-3-benzofuranyl)carbonyl]-2-methylphenoxy]-, methyl ester (CA INDEX NAME)

IT 139717-94-5P

RL: SPN (Synthetic preparation); PREP (Preparation) (preparation of, as drug for uric acid excretion)

RN 139717-94-5 CAPLUS

CN Acetic acid, 2-[4-[(2-ethyl-6-nitro-3-benzofuranyl)carbonyl]-2-methylphenoxy]- (CA INDEX NAME)



L25 ANSWER 11 OF 15 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1985:575270 CAPLUS <u>Full-text</u>

DOCUMENT NUMBER: 103:175270

ORIGINAL REFERENCE NO.: 103:28131a,28134a

TITLE: Antibacterial activity and polarographic half-wave

reduction potential of 2-nitrobenzo[b]furans AUTHOR(S):

Ohishi, Yoshitaka; Kuriyama, Kiyoshi; Doi, Yoshio;

Nakanishi, Teruo

CORPORATE SOURCE: Kyoto Res. Inst., Kaken Pharm. Co., Ltd., Kyoto, 607,

Japan

SOURCE: Chemical & Pharmaceutical Bulletin (1985), 33(7),

2854-61

CODEN: CPBTAL; ISSN: 0009-2363

DOCUMENT TYPE: Journal LANGUAGE: English

GΙ

AΒ The antibacterial activities of a series of derivs. of 2-nitrobenzo[b]furan (I) against Staphylococcus aureus, Bacillus subtilis, Escherichia coli, Salmonella typhimurium, Salmonella enteritidis, Shigella flexneri, Proteus vulgaris, or Pseudomonas aeruginosa were determined in vitro. Most of the compds. showed considerable activities against the bacteria except P. vulgaris and P. aeruginosa and 1 of them was .apprx.30-fold as active as nitrofurantoin against S. aureus. Mono- and dimethoxy derivs. were the most active. The polarog. half-wave potentials (E1/2) of the derivs. of I at pH 7 were in a narrow range of -0.450 ± 0.04 V, whereas the E1/2 values of regioisomeric nitrobenzo[b] furans were more neg. (-0.560 to -0.726 V). In the case of derivs. of I, substituent(s) on the benzene ring had little influence on the reduction potential of the 2-nitro group, whereas the antibacterial activity depended markedly on the substituent group(s).

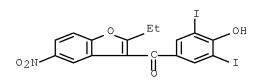
29735-83-9 98873-72-4 ΙT

> RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(bacteria sensitivity to)

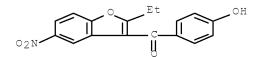
29735-83-9 CAPLUS RN

Methanone, (2-ethyl-5-nitro-3-benzofuranyl)(4-hydroxy-3,5-diiodophenyl)-CN (CA INDEX NAME)



98873-72-4 CAPLUS RN

Methanone, (2-ethyl-5-nitro-3-benzofuranyl)(4-hydroxyphenyl)- (CA INDEX CN NAME)



L25 ANSWER 12 OF 15 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1984:454904 CAPLUS Full-text

DOCUMENT NUMBER: 101:54904 ORIGINAL REFERENCE NO.: 101:8525a,8528a

TITLE: Benzarone derivatives and their use in treating venous

and arterial ailments

INVENTOR(S): Grote, Heinfried; Sandrock, Klaus

PATENT ASSIGNEE(S): Fed. Rep. Ger. SOURCE: Ger. Offen., 13 pp.

CODEN: GWXXBX

DOCUMENT TYPE: Patent LANGUAGE: German

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

| PATENT NO. | KIND | DATE | APPLICATION NO. | DATE |
|------------------------|--------|-----------|-----------------|----------|
| | | | | |
| DE 3342624 | A1 | 19840329 | DE 1983-3342624 | 19831125 |
| PRIORITY APPLN. INFO.: | | | DE 1983-3342624 | 19831125 |
| OTHER SOURCE(S): | MARPAT | 101:54904 | | |

GΙ

- AΒ The title compds. (I; R-R3 = H, alkoxy, acyloxy, OH, SO3H; R4 = H, acyl, HSO2), more effective than benzarone (II) (no data), were prepared Thus, II was acetylated to give 92% I (R-R3 = H, R4 = Ac). This was brominated with Nbromosuccinimide to give 100% I (R = R2 = R3 = H, R1 = Br, R4 = Ac). This was treated with CsOAc to give 100% I (R = R2 = R3 = H, R1 = OAc, R4 = Ac), which was saponified to give 48.8% I (R = R2 = R3 = R4 = H, R1 = OH).
- ΙT 90908-76-2

RL: RCT (Reactant); RACT (Reactant or reagent) (reduction of)

90908-76-2 CAPLUS RN

CN Methanone, (2-ethyl-5-nitro-3-benzofuranyl)(4-methoxyphenyl)- (CA INDEX NAME)

L25 ANSWER 13 OF 15 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1974:505428 CAPLUS $\underline{\text{Full-text}}$

DOCUMENT NUMBER: 81:105428

ORIGINAL REFERENCE NO.: 81:16679a,16682a

TITLE: Nitro derivatives of biological interest. IX.

Synthesis of 2-nitramino pyrimidines from chromones

and benzofurans

AUTHOR(S): Pene, Cecile; Hubert-Habart, Michel; Royer, Rene

CORPORATE SOURCE: Fond. Curie, Inst. Radium, Paris, Fr.

SOURCE: European Journal of Medicinal Chemistry (1974), 9(2),

202 - 4

CODEN: EJMCA5; ISSN: 0223-5234

DOCUMENT TYPE: Journal LANGUAGE: French

GI For diagram(s), see printed CA Issue.

AB Nitraminopyrimidines I (R = H, NO2; R1 = H, Et, Ph, NH2) were prepared in 56-99% yield by treating the benzofurans II (R2 = CHO, CH(OAc)2, COEt, Bz, CN) with nitroguanidine. III (R1 = H, Ph; R3 = H, Me) similarly were prepared from the chromones IV. Treatment of I and III with N2H4 gave 2-

hydrazinopyridines, which with NaNO2 gave either 2-azidopyrimidines or tetrazolopyrimi-dines.

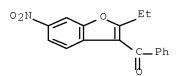
IT 42901-90-6

RL: RCT (Reactant); RACT (Reactant or reagent)

(reaction of, with nitroguanidine)

RN 42901-90-6 CAPLUS

CN Methanone, (2-ethyl-6-nitro-3-benzofuranyl)phenyl- (CA INDEX NAME)



L25 ANSWER 14 OF 15 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1973:505183 CAPLUS Full-text

DOCUMENT NUMBER: 79:105183

ORIGINAL REFERENCE NO.: 79:17058h,17059a

TITLE: Nitro derivatives of biological interest. VI.

Synthesis of 5-(2-hydroxy-4-nitrophenyl) pyrimidines from nitro derivatives of benzofurans substituted in

the 3-position by an electroattractive group

AUTHOR(S): Hubert-Habart, Michel; Pene, Cecile; Bastian, Gerard;

Royer, Rene

CORPORATE SOURCE: Serv. Chim., Fond. Curie-Inst. Radium, Paris, Fr.

SOURCE: Chimica Therapeutica (1973), 8(3), 314-18

CODEN: CHTPBA; ISSN: 0009-4374

DOCUMENT TYPE: Journal LANGUAGE: French

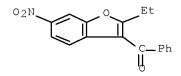
GI For diagram(s), see printed CA Issue.

AB Pyrimidines I (R = H, Me, Et, Ph, NH2; R1 = NH2, Me) were prepared in 70-90% yield and II (X = O, S) in 9-99% yield by nitrating the benzofurans III (R2 = CHO, Ac, COEt, COPh, CN; R3 = H) in 43-60% yield and treating III (R3 = NO2) with R1C(:NH)NH2 or CX(NH2)2.

IT 42901-90-6P

RN 42901-90-6 CAPLUS

CN Methanone, (2-ethyl-6-nitro-3-benzofuranyl)phenyl- (CA INDEX NAME)



L25 ANSWER 15 OF 15 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 1970:516689 CAPLUS <u>Full-text</u>

DOCUMENT NUMBER: 73:116689

ORIGINAL REFERENCE NO.: 73:18989a,18992a

TITLE: Inhibitory action of benzofuran compounds on 5'-AMP

deaminase and adenosine deaminase

AUTHOR(S): Nakanishi, Teruo; Saeki, Toru

CORPORATE SOURCE: Res. Lab., Kakenyaku-Kako Co., Ltd., Japan

SOURCE: Seikagaku (1970), 42(6), 286-90

CODEN: SEIKAQ; ISSN: 0037-1017

DOCUMENT TYPE: Journal LANGUAGE: Japanese

AB The inhibitory action of benzofuran derivs. on 5'-AMP deaminase (I) and adenosine deaminase (II) was investigated by using a number of synthetic compds. Introduction of carboxyl or hydroxyl groups increased the inhibitory action on I, but no pronounced effect of the substituent was observed on II. No common feature in structure seems to exist for the inhibition of these 2 deaminases.

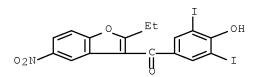
IT 29735-83-9

RL: BIOL (Biological study)

(adenylate deaminase inhibition by)

RN 29735-83-9 CAPLUS

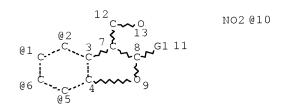
CN Methanone, (2-ethyl-5-nitro-3-benzofuranyl)(4-hydroxy-3,5-diiodophenyl)- (CA INDEX NAME)



FILE 'HOME' ENTERED AT 09:54:16 ON 23 DEC 2008

SEARCH HISTORY

=> d stat que 116; d his nofile L5 STR



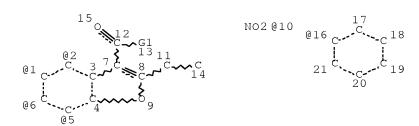
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GRAPH ATTRIBUTES: RSPEC I

NUMBER OF NODES IS 13

STEREO ATTRIBUTES: NONE

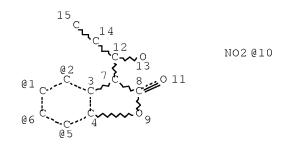
L8 129 SEA FILE=REGISTRY SSS FUL L5
L9 STR



VAR G1=OH/X/16 VPA 10-1/2/5/6 U NODE ATTRIBUTES: DEFAULT MLEVEL IS ATOM DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RSPEC I
NUMBER OF NODES IS 21

STEREO ATTRIBUTES: NONE L11 STR



VPA 10-1/2/5/6 U
NODE ATTRIBUTES:
CONNECT IS E3 RC AT 12
CONNECT IS E1 RC AT 13
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:

RSPEC I

NUMBER OF NODES IS 15

STEREO ATTRIBUTES: NONE

L16 57 SEA FILE=REGISTRY SUB=L8 SSS FUL (L9 OR L11)

100.0% PROCESSED 59 ITERATIONS 57 ANSWERS

SEARCH TIME: 00.00.01

(FILE 'HOME' ENTERED AT 09:40:20 ON 23 DEC 2008)

FILE 'CAPLUS' ENTERED AT 09:40:37 ON 23 DEC 2008 E US2006-584440/APPS

L1 1 SEA SPE=ON ABB=ON US2006-584440/AP D SCAN

SEL RN

FILE 'REGISTRY' ENTERED AT 09:41:11 ON 23 DEC 2008

L2 9 SEA SPE=ON ABB=ON (100-66-3/BI OR 108-90-7/BI OR 141627-42-1/BI OR 141645-16-1/BI OR 349102-73-4/BI OR 856758-02-6/BI OR 856758-03-7/BI OR 856758-04-8/BI OR 856758-05-9/BI)

D SCAN

L3 STR

L4

6 SEA SSS SAM L3

D SCAN

L5 STR L3

L6 5 SEA SSS SAM L5

L7 2417 SEA SSS FUL L5 EXTEND

L8 129 SEA SSS FUL L5

SAVE TEMP L8 CHA440FULL/A

L9 STR L5

L10 0 SEA SSS SAM L9

L11 STR L5

L12 0 SEA SSS SAM L11

L13 0 SEA SUB=L8 SSS SAM (L9 OR L11)

| L14 L15 L16 | | | |
|---|---|--|--|
| L18 L19 L20 L21 L22 L23 L24 | 4 SEA SPE=ON ABB=ON BLEGER F?/AU 2 SEA SPE=ON ABB=ON MORDACQ F?/AU 67 SEA SPE=ON ABB=ON PIRON J?/AU D BIB L1 | | |
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| | FILE 'REGISTRY' ENTERED AT 09:53:57 ON 23 DEC 2008 D STAT QUE L16 | | |
| L25 | FILE 'CAPLUS' ENTERED AT 09:53:57 ON 23 DEC 2008 D QUE NOS L18 15 SEA SPE=ON ABB=ON L18 NOT L24 D IBIB ABS HITSTR L25 1-15 | | |
| | FILE 'HOME' ENTERED AT 09:54:16 ON 23 DEC 2008 D STAT QUE L16 | | |

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